Non-hermitian physics in strongly electron systems

CCSE, Japan Atomic Energy Agency (JAEA)
RIKEN AIP

Yuki Nagai

Collaborators

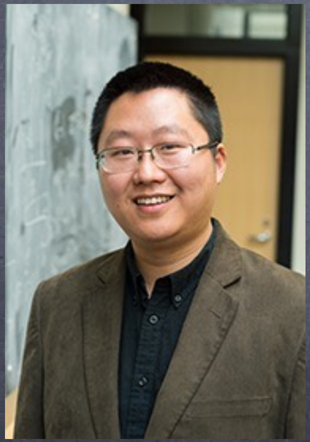
Yuki Nagai[1], Yang Qi[2], Hiroki Isobe[3], Vladyslav Kozii[3], and Liang Fu[3]

submitted

[1]CCSE, Japan Atomic Energy Agency, Japan

[2]Department of Physics, Fudan University, China

[3]Department of Physics, Massachusetts Institute of Technology, USA



Liang Fu's group in MIT

Yang Qi in Fudan Univ in China

I was a one-year visiting researcher in MIT (2016-2017)

This project started when Yang and I were in MIT

Outline

- Non-hermitian topological theory in strongly correlated systems in finite temperature
- Heavy fermions systems and Bulk Femi arcs
- Summary

Yuki Nagai[1], Yang Qi[2], Hiroki Isobe[3], Vladyslav Kozii[3], and Liang Fu[3]

[1]CCSE, Japan Atomic Energy Agency, Japan

[2]Department of Physics, Fudan University, China

[3]Department of Physics, Massachusetts Institute of Technology, USA

submitted

Non-hermitian topological theory in strongly correlated systems in finite temperatures

Non-hermitian "Hamiltonian"

$$H(\mathbf{k},\omega) \equiv H_0(\mathbf{k}) + \Sigma(\mathbf{k},\omega)$$

Quantum theory of solids

Schrodinger eq. in solids

$$H(r,-i\nabla)\psi(r) = E\psi(r)$$

Solid: periodic potential

Bloch wave functions

$$\psi_k(r) = \exp[ikr]u_k(r)$$

$$u_k(r+L) = u_k(r)$$

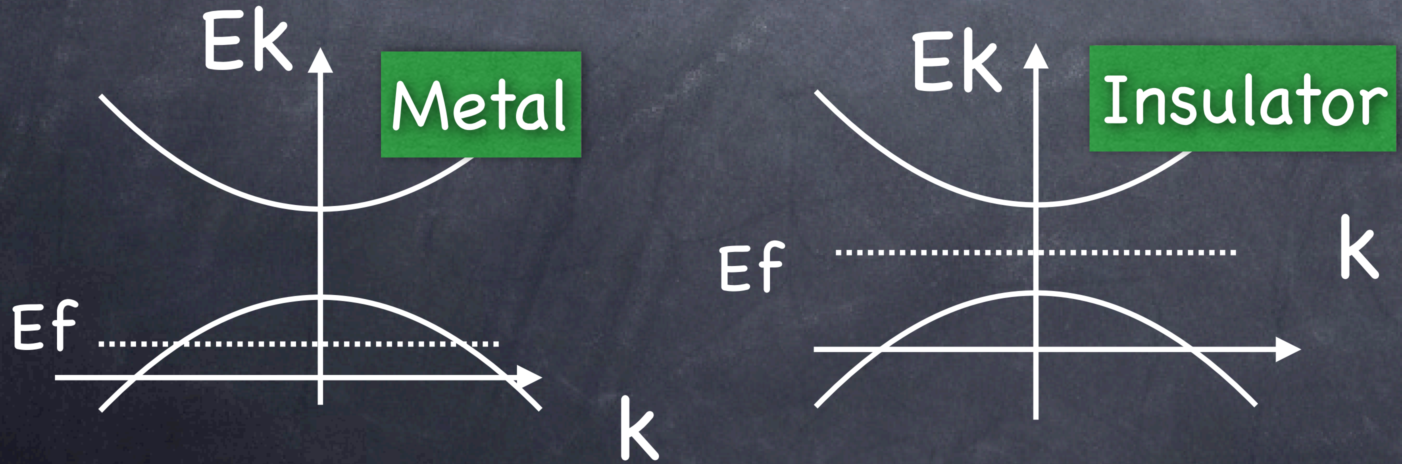
Band theory

$$H_k(r,-i\nabla)\psi_k(r) = E_k\psi_k(r)$$

E_k eigenvalues

Ef: Fermi energy

Fermi "sea" level



Quantum theory of solids

Topological Band theory   Thouless et al(1982), Haldane (1988) etc.

For example   **Topological insulator**

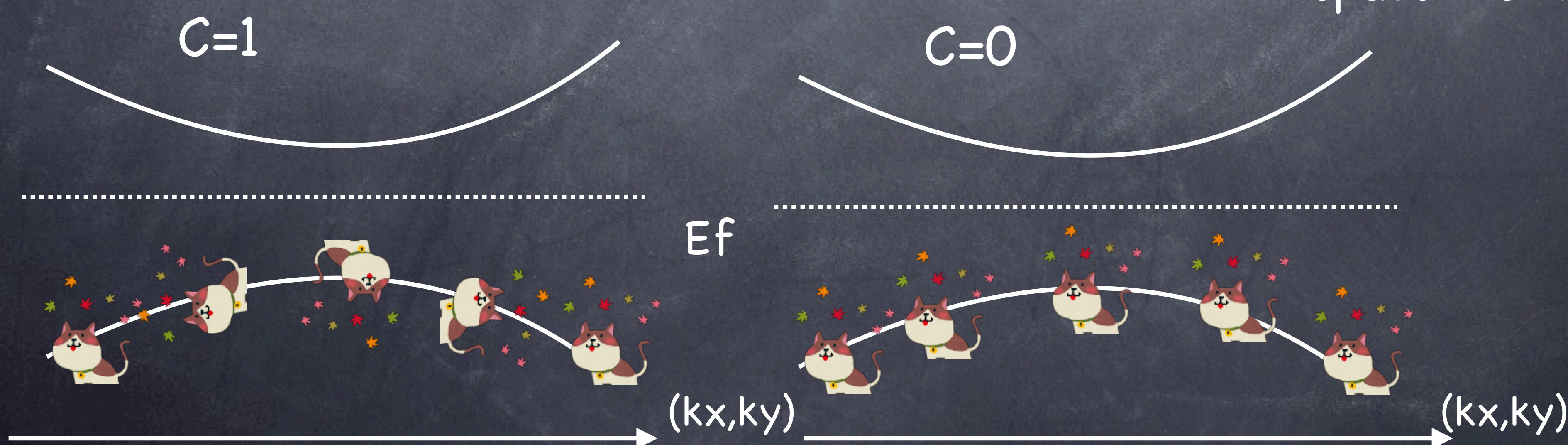
$H_k|\psi_k\rangle = E_k|\psi_k\rangle$ $|\psi_k\rangle$ wavefunction for a filled band (Ek < Ef)

Berry connection $A = \langle \psi_k | \nabla_k \psi_k \rangle$

Chern number $C = \int dk_x dk_y (\mathrm{rot} A(k))_z$

 $\sim |\psi_k\rangle$

k-space: 2D torus



Green's functions

Physical observables can be calculated by Green's functions

Green's function for operators A and B: $G_{AB} = \langle AB \rangle$

For example: one-particle Green's function

$$G(\tau) = \langle T_\tau \psi(\tau) \psi^\dagger(0) \rangle$$

We can calculate the density of states from this Green's function

We do not need to know wavefunctions to calculate physical observables!

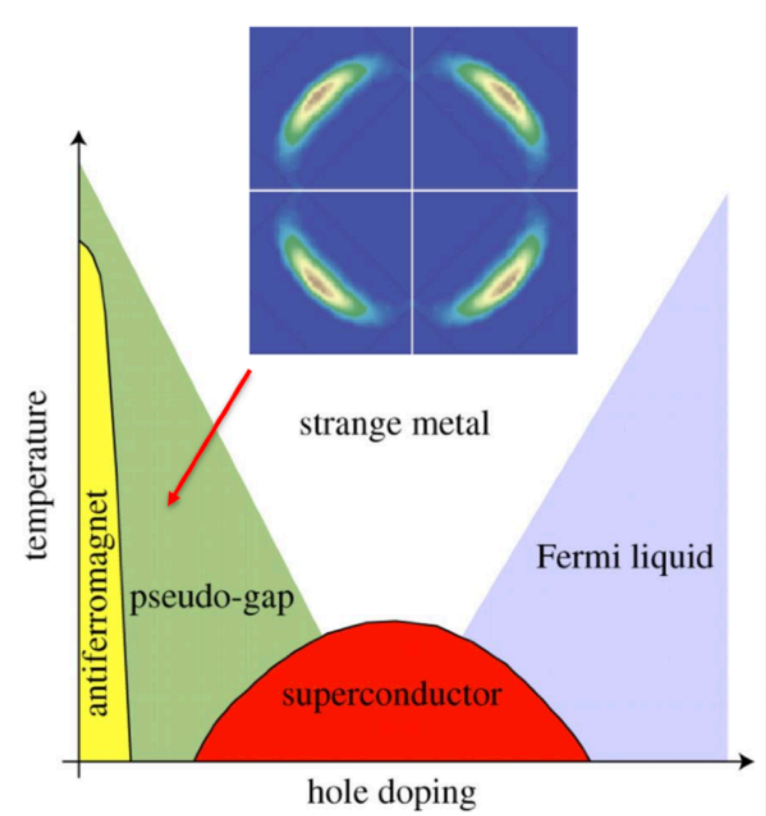
Topology? $N_2 = \frac{1}{24\pi^2} \int dk_0 d^2 \vec{k}^2 \mathrm{Tr} \left[\epsilon^{\mu\nu\rho} \hat{G} \frac{\partial \hat{G}^{-1}}{\partial \mu} \hat{G} \frac{\partial \hat{G}^{-1}}{\partial \nu} \hat{G} \frac{\partial \hat{G}^{-1}}{\partial \rho} \right]$

Chern number

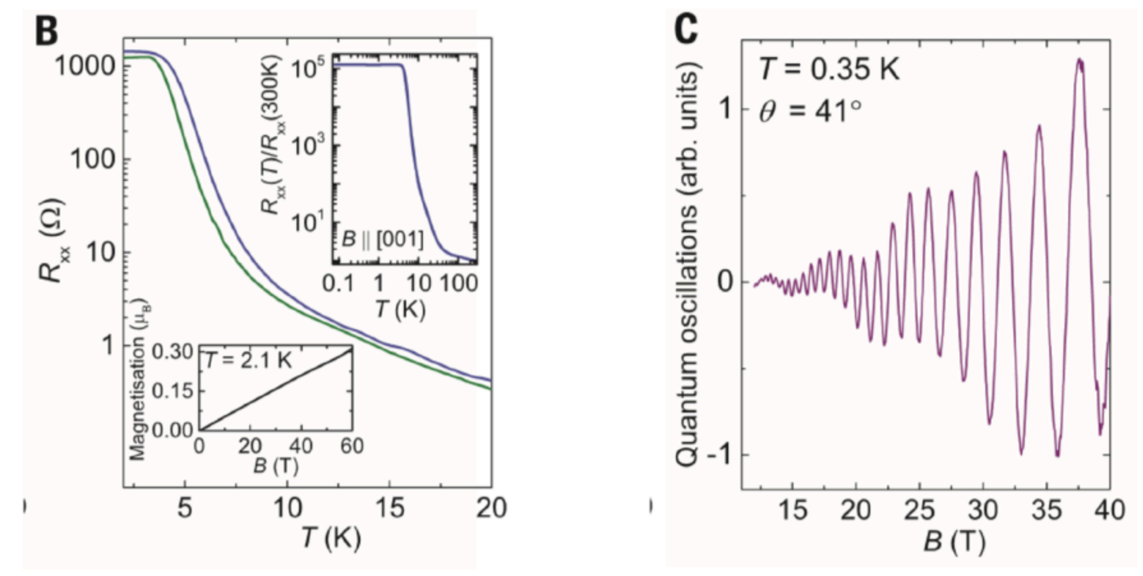
Green's function can be defined in strongly correlated systems with finite temperature

New topological theory

Interesting phenomena in correlated electron systems



Fermi arc in cuprates



Sebastian et al, Science (2015); Li et al, Science (2014)

SmB_6 and YbB_{12} : "Fermi surface" in Kondo insulators

There might be "topology" in correlated electron systems, which might explain these phenomena

Non interacting systems

Hamiltonian H_0

Schrodinger eq.

$$H_0|i\rangle = E_i|i\rangle$$

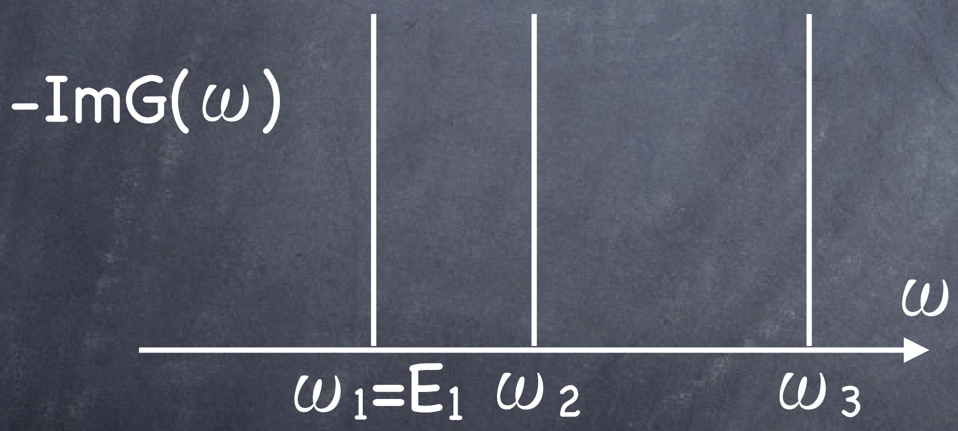
One-particle Green's function

$$G^R(\omega) = \left[\omega - H_0\right]^{-1}$$

Poles: $\det\left[\omega_i - H_0\right] = 0$

-> Poles are at $\omega = E_i$

Poles are on real axis because
H_0 is a hermitian matrix



What happens in interacting systems?

Interacting systems

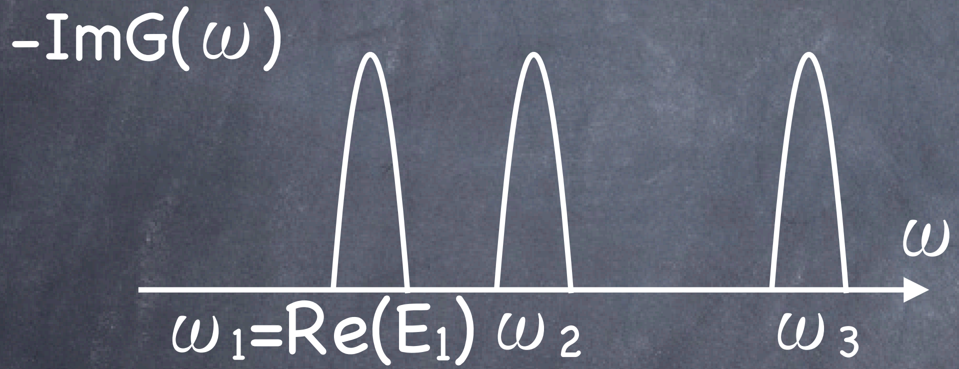
Hamiltonian

$$H = H_0 + H_I$$

One-particle Green's function

$$G^R(\omega) = \left[\omega - H_0 - \Sigma(\omega)\right]^{-1}$$

Σ: self-energy



Poles: $\det\left[\omega_i - H_0 - \Sigma(\omega_i)\right] = 0$

If the self-energy does not depend on the energy: Σ=const.

Poles: $\det\left[\omega_i - H_{\mathrm{eff}}\right] = 0$

We can define <u>effective</u> Hamiltonian: $H_{\mathrm{eff}} \equiv H_0 + \Sigma$

Poles are on complex plane because <u>H_{eff} is a non-hermitian matrix</u>

$$H_{\mathrm{eff}}|i\rangle = E_i|i\rangle$$

Quasiparticle damping and dispersion

Green's function: $G^R(\mathbf{k}, \omega) = (\omega - H_{\text{eff}}(\mathbf{k}))^{-1}$

Quasiparticle Hamiltonian: $H_{\text{eff}}(\mathbf{k}) \equiv H_0(\mathbf{k}) + \Sigma(\mathbf{k})$

(non-Hermitian)

Bloch Hamiltonian

Self-energy

Finite lifetime means $\sum$ is **non-Hermitian:** $\Sigma = \Sigma' + i\Sigma'$

Poles of G^R in complex plane determines

$\text{Re}(E_{\mathbf{k}})$ quasiparticle dispersion

$\text{Im}(E_{\mathbf{k}})$ inverse lifetime

single-band system: $E_k = \epsilon_k - i\gamma_k$

Quasiparticle damping and dispersion

Green's function: $G^R(\mathbf{k},\omega) = (\omega - H_{\text{eff}}(\mathbf{k}))^{-1}$

Quasiparticle Hamiltonian: $H_{\text{eff}}(\mathbf{k}) \equiv H_0(\mathbf{k}) + \Sigma(\mathbf{k})$

(non-Hermitian)

Bloch Hamiltonian | Self-energy

Finite lifetime means $\sum$ is **non-Hermitian:** $\Sigma = \Sigma' + i\Sigma'$

Poles of G^R in complex plane determines

$\text{Re}(E_{\mathbf{k}})$ quasiparticle dispersion

$\text{Im}(E_{\mathbf{k}})$ inverse lifetime

multi-orbital systems: H_0 and Σ are matrices and generally do not commute

=> damping can dramatically alter qp dispersion in zero/small-gap systems

Damping reshapes dispersion

Quasiparticles in zero/small gap systems

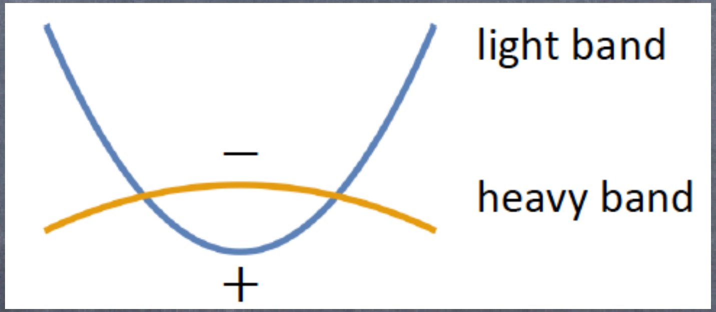
Bloch Hamiltonian + self-energy with **two lifetimes**

2D system with linear dispersion (Dirac cone)

$$H_0(\mathbf{k}) = \begin{pmatrix} \epsilon_{1k} & V_k \\ V_k^* & \epsilon_{2k} \end{pmatrix} \sim \begin{pmatrix} v_1 k_x & v_y k_y \\ v_y p_y & -v_2 k_x \end{pmatrix}$$

near hybridization nodes

$$\Sigma = \begin{pmatrix} i\Gamma_1 & 0 \\ 0 & i\Gamma_2 \end{pmatrix}$$



Point nodes on kx axis protected by reflection y -> -y

Two orbitals unrelated by symmetry generally have different lifetimes

Example: d- and f-orbitals in heavy fermion systems.

Kozii and Fu, arxiv:1708.05841

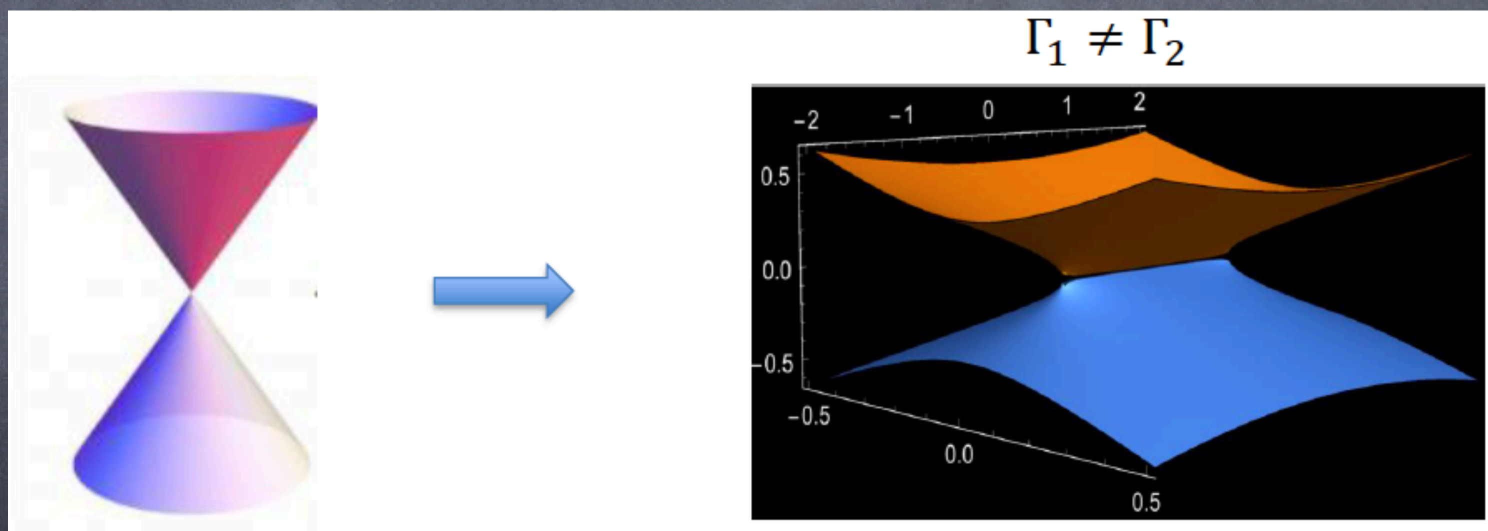
Asymmetric damping reshapes dispersion

Go back to a simple case

Quasiparticle Hamiltonian

$$H(\mathbf{k}) = \begin{pmatrix} v_1 k_x - i\Gamma_1 & v_y k_y \\ v_y p_y & -v_2 k_x - i\Gamma_2 \end{pmatrix}$$

Quasiparticle dispersion $\mathrm{Re}(E_k)$:



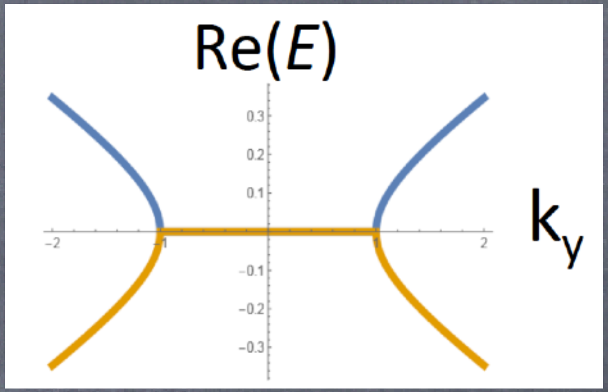
$\Gamma_1 - \Gamma_2 \neq 0$: two bands stick together to form an open nodal arc, terminating at $k_x = 0$, $k_y = \pm(\Gamma_1 - \Gamma_2)/2v_y$

Extreme anisotropy

Bulk Fermi arc

Non-Hermitian quasiparticle Hamiltonian:

$$H(\mathbf{k}) = \begin{pmatrix} \epsilon_{1k} - i\Gamma_1 & V_k \\ V_k^* & \epsilon_{2k} - i\Gamma_2 \end{pmatrix}$$



Complex spectrum

$$E_\pm(\mathbf{k}, \omega) = \bar{\epsilon}_k \pm \sqrt{(\epsilon_{1k} - \epsilon_{2k} - i\gamma)^2 + |V_k|^2} - i\Gamma \qquad \text{where, } \Gamma, \gamma = (\Gamma_1 \pm \Gamma_2)/2$$

With hybridization and asymmetric damping $\gamma \neq 0$

for $|V_k| > \gamma : \mathrm{Re}\,(E_+) \neq \mathrm{Re}\,(E_-)$ (gap opens)

for $|V_k| < \gamma : \mathrm{Re}\,(E_+) = \mathrm{Re}\,(E_-) = 0$ (gap closes)

Level sticking instead of repulsion!

Near end of nodal arc, $\mathrm{Re}\,(E_+ - E_-) \propto \sqrt{k_y - k_0}$

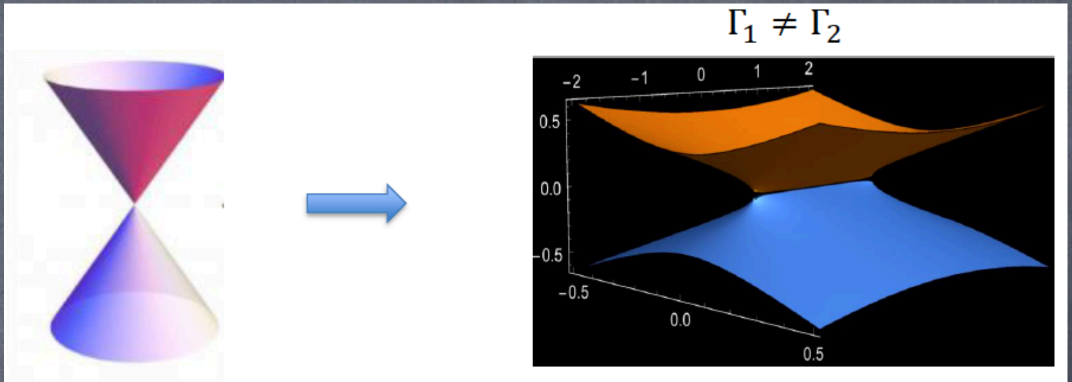
Topological index

Complex energy:

$$E_{\pm}(\mathbf{k},\omega) = \pm\sqrt{v_y^2 k_y^2 - \gamma^2} - i\Gamma$$

Quasiparticle Hamiltonian:

$$H(\mathbf{k}) = \begin{pmatrix} v_1 k_x - i\Gamma_1 & v_y k_y \\ v_y p_y & -v_2 k_x - i\Gamma_2 \end{pmatrix}$$



$\mathrm{Re}E_{\pm} = 0$

$|k_y| \leq \gamma/v_y \equiv k_0$

k_0:exceptional points

It only has a single eigenstate

$$\psi = (1,i)^T$$

Topological index: vorticity of complex energy "gap" in k-space

$$\nu_{nm}(\Gamma) = -\frac{1}{2\pi}\oint_{\Gamma} \nabla_{\mathbf{k}} \arg\left[E_m(\mathbf{k}) - E_n(\mathbf{k})\right] \cdot d\mathbf{k}$$

 $\sim E_m$ 

Topological charge: ν =±1/2

H. Shen, B. Zhen, and L. Fu, Phys. Rev. Lett. 120, 146402 (2018)

End of nodal arc: exceptional point

$$H(\mathbf{k}) = \begin{pmatrix} v_1 k_x - i\gamma & v_y k_y \\ v_y p_y & -v_2 k_x + i\gamma \end{pmatrix} - i\Gamma \rightarrow \begin{pmatrix} -i\gamma & \gamma \\ \gamma & i\gamma \end{pmatrix} - i\Gamma$$

at $\pm k_0 = (0, \pm\gamma/v_y)$

$$G^{\mathrm{R}}(k_0) = \frac{1}{(\omega - i\Gamma)^2} \begin{pmatrix} \omega - i\Gamma_2 & -\gamma \\ -\gamma & \omega - i\Gamma_1 \end{pmatrix}$$

at ends of Fermi arc $k = \pm k_0$, H is non-diagonalizable: has only one eigenstate!

This is a feature of **non-Hermitian** operator
(Two poles of Green's function merge into one)

Interacting systems

A self-energy usually has energy dependence

Linearly dependent case What happens?

One-particle Green's function

$$G^R(\omega) = \left[\omega - H_0 - \Sigma(\omega)\right]^{-1}$$

Σ: self-energy

Poles: $\det\left[\omega_i - H_0 - \Sigma(\omega_i)\right] = 0$

If $\Sigma = \Sigma_0 + \Sigma_1 \omega$,

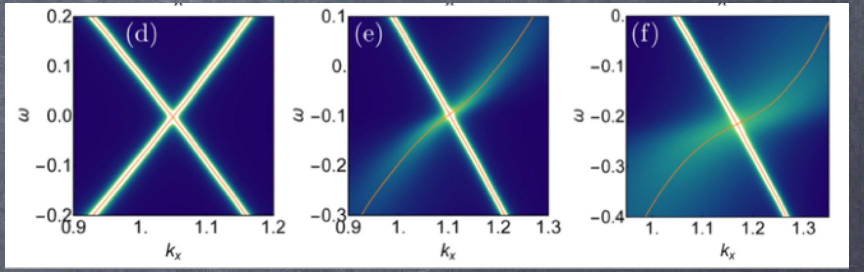
Poles: $\det\left[\omega_i - H_{\mathrm{eff}}\right] = 0$

$$H_{\mathrm{eff}} \equiv (1 - \Sigma_1)^{-1}(H_0 + \Sigma_0)$$

$(1 - \Sigma_1)^{-1}$ is a matrix

-> Orbital-dependent effect

2D disordered Dirac model



M. Papaj, H. Isobe and L. Fu, Phys. Rev. B 99, 201107(R)

Damping reshapes dispersion

We can also define the effective non-hermitian Hamiltonian

Preliminary

Interacting systems

A self-energy usually has energy dependence

$$G^R(\omega) = \left[\omega - H_0 - \Sigma(\omega)\right]^{-1}$$

More general case?

Polynomial expansion: $\Sigma(\omega) = \sum_{k=0}^{d} \omega^k \Sigma_k$

$$\det\left[\omega_i - H_0 - \Sigma(\omega_i)\right] = 0$$

→ lambda-matrix problem

J. E. Dennis Jr. et al., Tech. Rep. CMU-CS-71-110, Computer Science Department, Carnegie Mellon University, 1971.

$$\det\left[B\omega_i - H_{\mathrm{eff}}\right] = 0$$

Generalized eigenvalue problem

$$H_{\mathrm{eff}} = \begin{pmatrix} 0 & I & 0 & \cdots & 0 \\ 0 & 0 & I & 0 & \vdots \\ \vdots & \vdots & 0 & \ddots & \\ -H_0 - \Sigma_0 & I - \Sigma_1 & \cdots & -\Sigma_{d-2} & -\Sigma_{d-1} \end{pmatrix}$$

A companion matrix

$$B = \mathrm{diag}(I, I, \cdots, -\Sigma_d)$$

Topology for generalized eigenvalue problem?

Microscopic origins of two lifetimes

Electron-phonon interaction:

Kozii and Fu, arxiv:1708.05841

two orbitals with different e-ph coupling constants

Electron-electron interaction:

This talk, YN et al. submitted

periodic Anderson model

$$\mathscr{H} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} f^\dagger_{\mathbf{k}\sigma} & c^\dagger_{\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} \epsilon_{f\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}} & \epsilon_{c\mathbf{k}} \end{pmatrix} \begin{pmatrix} f_{\mathbf{k}\sigma} \\ c_{\mathbf{k}\sigma} \end{pmatrix} + U \sum_i f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow}$$

interaction of f-electron only $\Sigma = \begin{pmatrix} -i\Gamma & 0 \\ 0 & 0 \end{pmatrix}$

This talk and related poster

This talk

Prediction: bulk Fermi arc in heavy fermion systems

Heavy-fermion system **naturally** features two lifetimes, since there are two kinds of electrons, **itinerant** c-electrons and **localized** f-electrons

We focus on Kondo semimetal

Related poster

Disorder-induced Weyl exceptional ring and spectral collapse of Landau levels in Weyl semimetals

Taiki Matsushita, YN, Satoshi Fujimoto

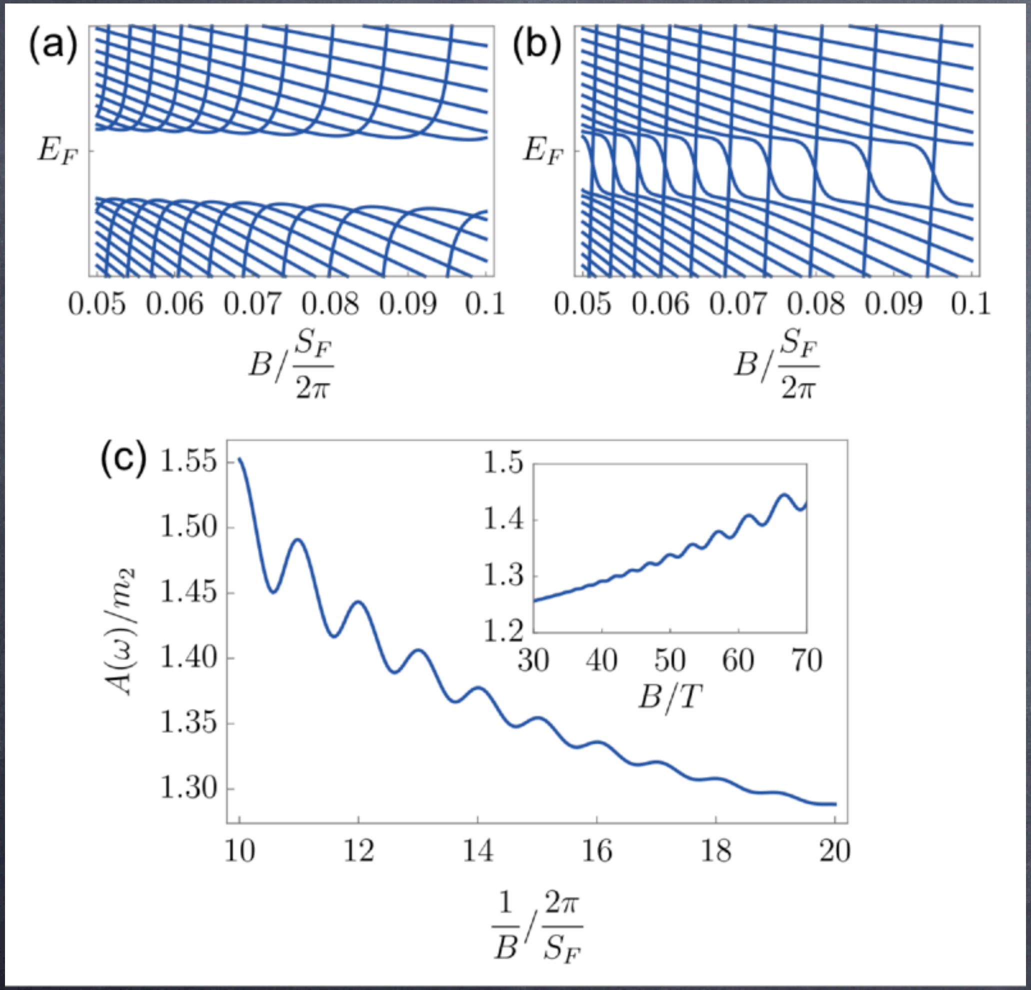
Non-Hermitian phenomena in disordered WSMs are discussed

General scheme for a generation of WERs

Taiki Matsushita, YN, S. Fujimoto arXiv:1908.03345 (2019).

Insulator's Fermi surface

H. Shen and L. Fu, Phys. Rev. Lett. 121, 026403 (2018)



Landau level renormalized by damping

in-gap density of states exhibits quantum oscillation with periodicity set by kf

weak disorder => small mass

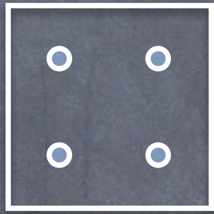
weak disorder => finite lifetime
=> non-Hermitian Landau level
=> quantum oscillation

Heavy fermions systems and Bulk Femi arcs

Kondo semimetal

Kondo insulator with a momentum-dependent hybridization gap

e.g. CeNiSn



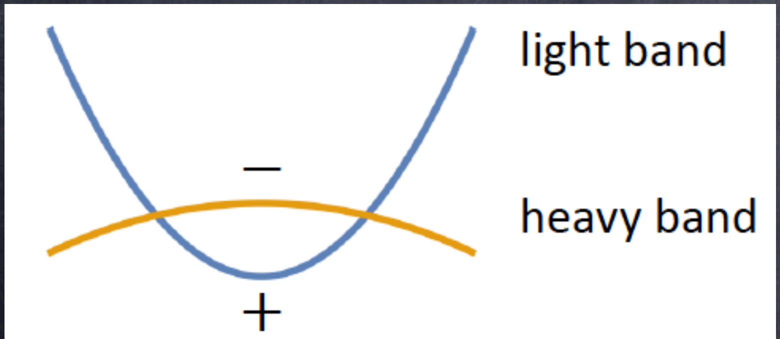
4 Dirac cones

Model: Periodic Anderson model

$$\mathscr{H} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} f^{\dagger}_{\mathbf{k}\sigma} & c^{\dagger}_{\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} \epsilon_{f\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}} & \epsilon_{c\mathbf{k}} \end{pmatrix} \begin{pmatrix} f_{\mathbf{k}\sigma} \\ c_{\mathbf{k}\sigma} \end{pmatrix} + U \sum_i f^{\dagger}_{i\uparrow} f_{i\uparrow} f^{\dagger}_{i\downarrow} f_{i\downarrow}$$

c-electron: $\epsilon_{c\mathbf{k}} = -2t(\cos k_x + \cos k_y)$

f-electron: $\epsilon_{f\mathbf{k}} = 0$ d-wave Hybridization: $v_{\mathbf{k}} = v(\cos k_x - \cos k_y)$



f-electrons feel strong e-e interaction

$$\Sigma = \begin{pmatrix} -i\Gamma & 0 \\ 0 & 0 \end{pmatrix}$$

Complex energy

Quasiparticle complex energy

$$E_\pm(\mathbf{k},\omega) = \pm\frac{1}{2}\sqrt{(M_\mathbf{k} - i\Gamma)^2 + 4\,|\,v_\mathbf{k}\,|^2} + \frac{1}{2}(\epsilon_{f\mathbf{k}} - i\Gamma + \epsilon_{c\mathbf{k}})$$

$$M_\mathbf{k} = \epsilon_{f\mathbf{k}} - \epsilon_{c\mathbf{k}}$$

Spectral function

$$\rho(\mathbf{k},\omega) = -\frac{2}{\pi}\left[\frac{1}{\omega - E_+(\mathbf{k},\omega)} + \frac{1}{\omega - E_-(\mathbf{k},\omega)}\right]$$

Focusing on the line M_k=0

$$E_\pm(\mathbf{k},\omega) = \pm\frac{1}{2}\sqrt{-\Gamma^2 + 4\,|\,v_\mathbf{k}\,|^2} - i\frac{\Gamma}{2}$$

Topological exceptional points appear at $\Gamma=2|v_k|$

Where are EPs in momentum space?

A. Near Dirac point on this line

Bulk Fermi arcs

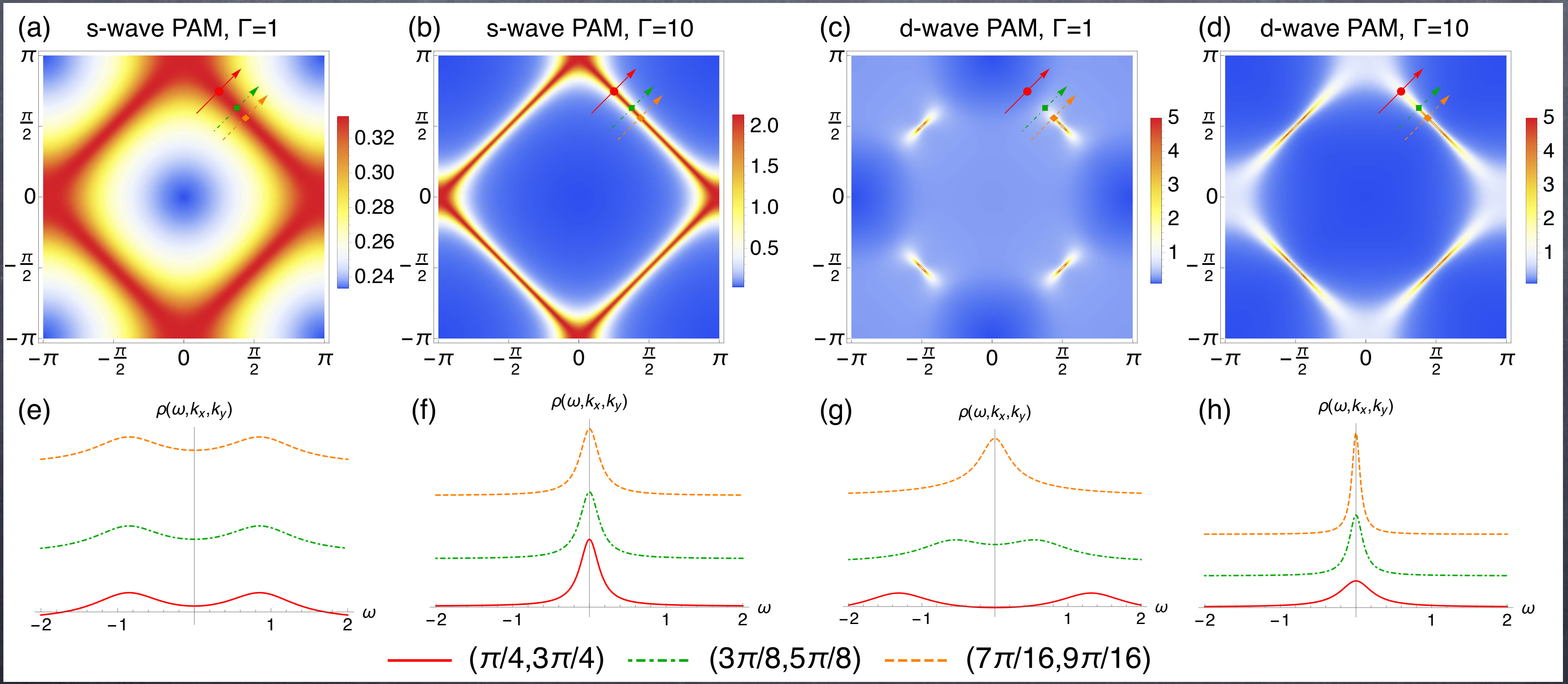
$$E_{\pm}(\mathbf{k},\omega) = \pm\frac{1}{2}\sqrt{-\Gamma^2 + 4|v_{\mathbf{k}}|^2} - i\frac{\Gamma}{2}$$

$$\rho(\mathbf{k},\omega) = -\frac{2}{\pi}\left[\frac{1}{\omega - E_{+}(\mathbf{k},\omega)} + \frac{1}{\omega - E_{-}(\mathbf{k},\omega)}\right]$$

Let us put the quasiparticle lifetime by **hand**

Kondo insulator

Kondo semimetal



Bulk Fermi arcs appear in d-wave PAM

Numerical confirmation

Model: Periodic Anderson model

$$\mathscr{H} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} f^\dagger_{\mathbf{k}\sigma} & c^\dagger_{\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} \epsilon_{f\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}} & \epsilon_{c\mathbf{k}} \end{pmatrix} \begin{pmatrix} f_{\mathbf{k}\sigma} \\ c_{\mathbf{k}\sigma} \end{pmatrix} + U \sum_i f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow}$$

We solve this model numerically

Dynamical mean-field theory (DMFT) with continuous-time quantum Monte Carlo impurity solver

Open-source program package iQIST is used

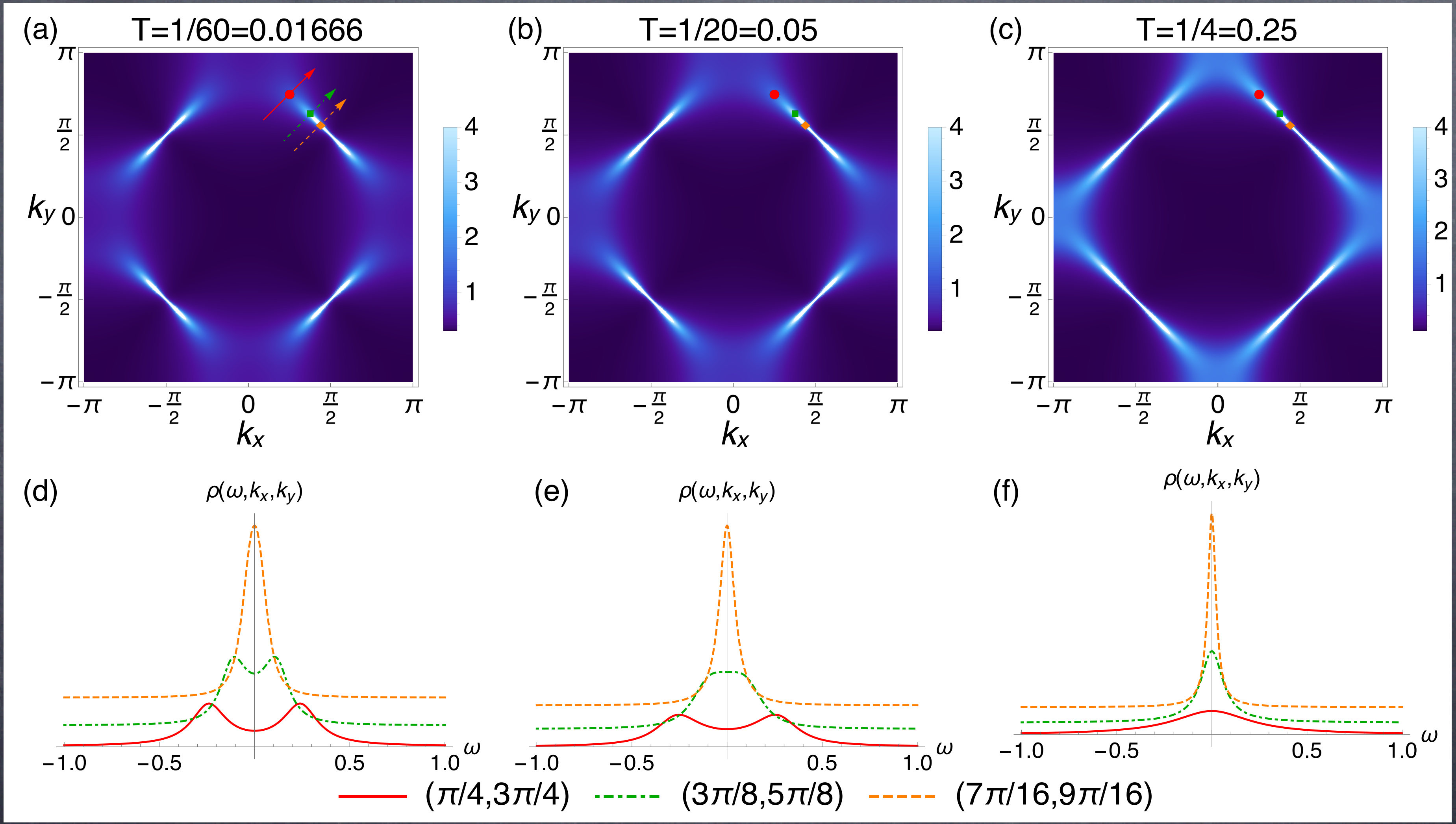
L. Huang et al., Compt. Phys. Commun. 195, 140 (2015)

The self-energy depends on temperature

-> The length of the bulk Fermi arc depends on temperature

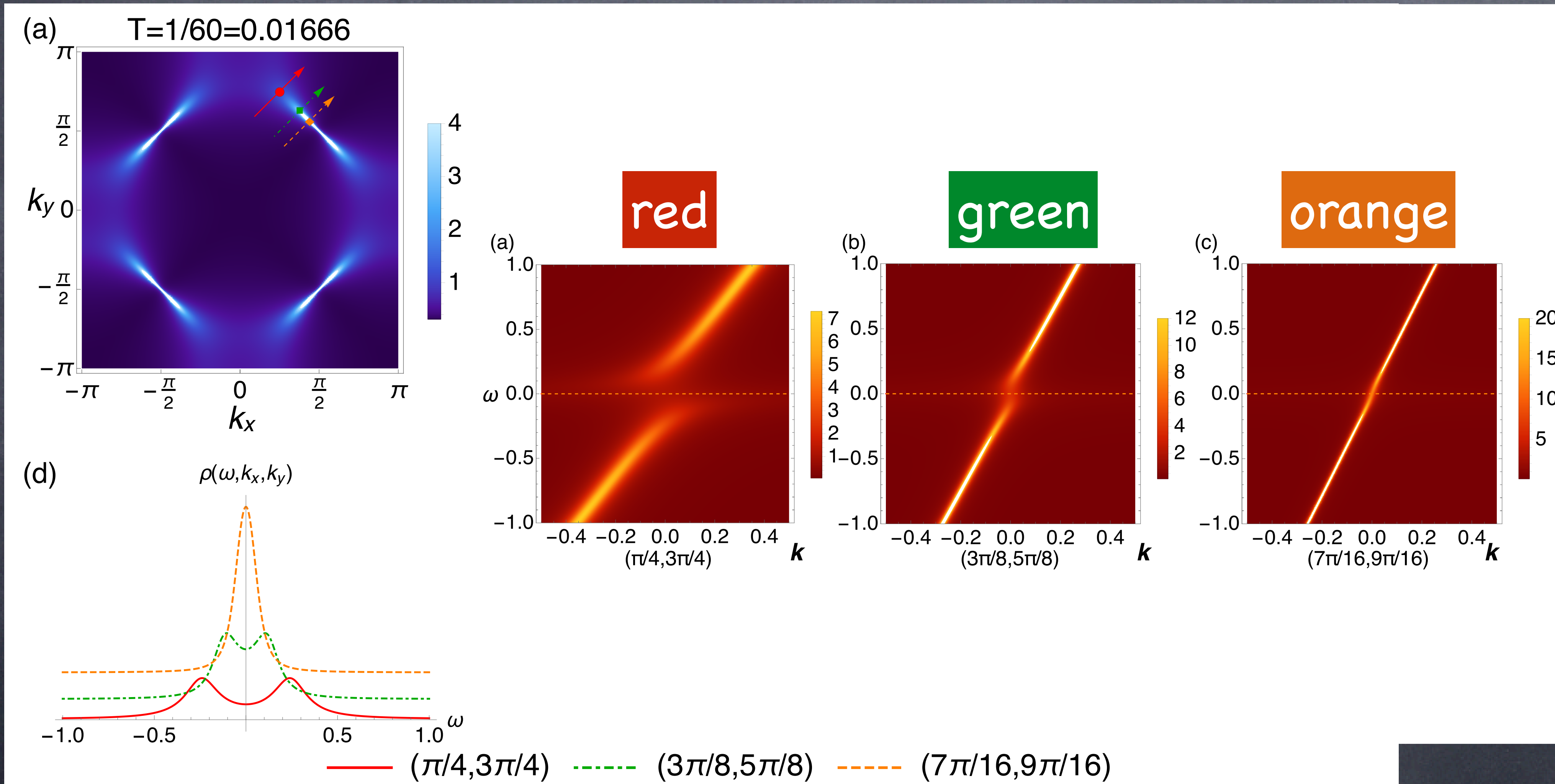
Numerical analytic continuation is done by the Pade approximation

DMFT results



The bulk Fermi arc appears depends on temperature

DMFT results

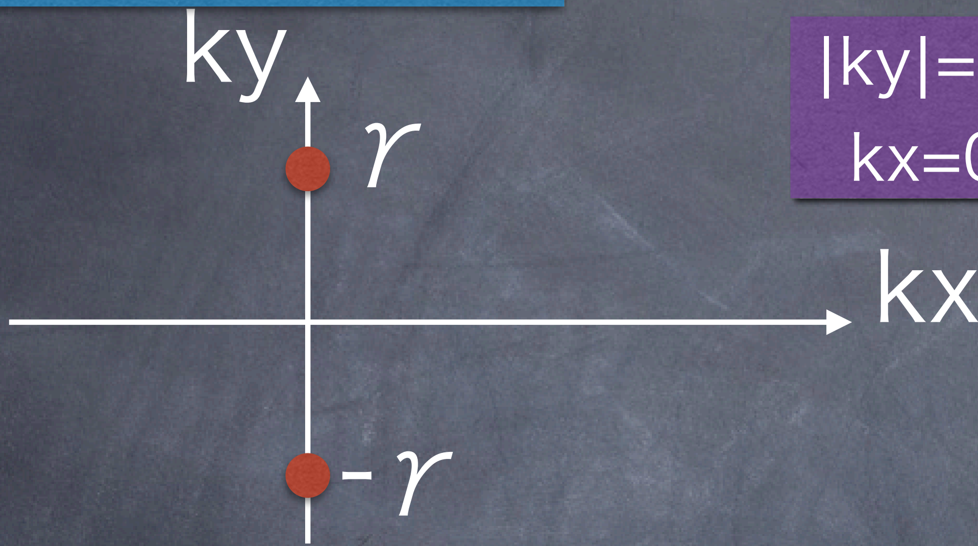


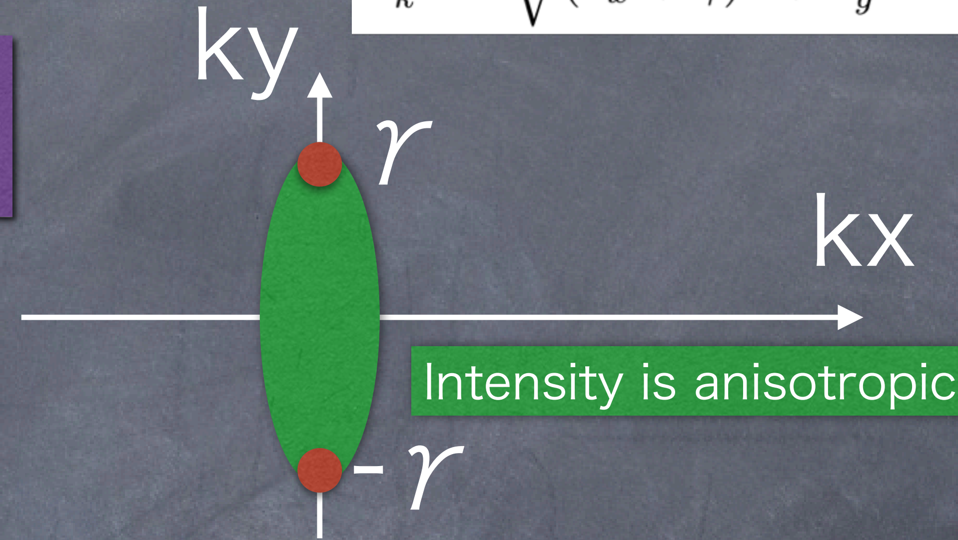
The bulk Fermi arc appears
depends on temperature

Exceptional points

2D Dirac Model

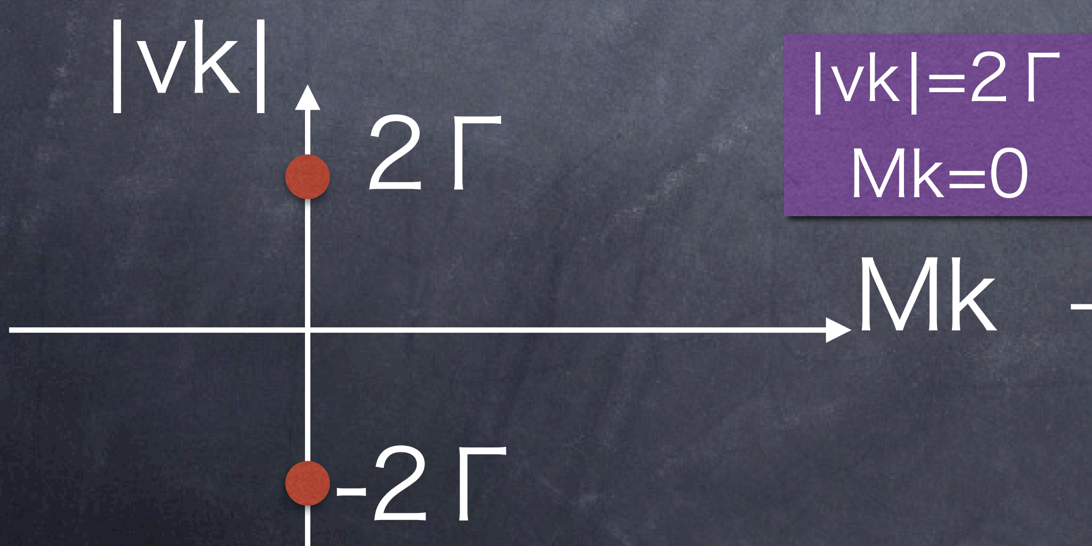
$$E_k^{\mathrm{eff}} = \sqrt{(k_x+\gamma)^2 + k_y^2} - i\Gamma$$

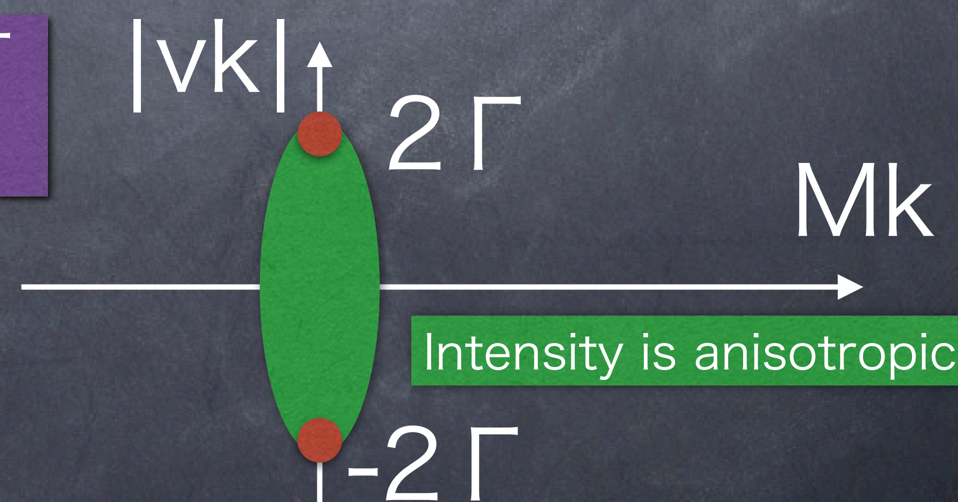




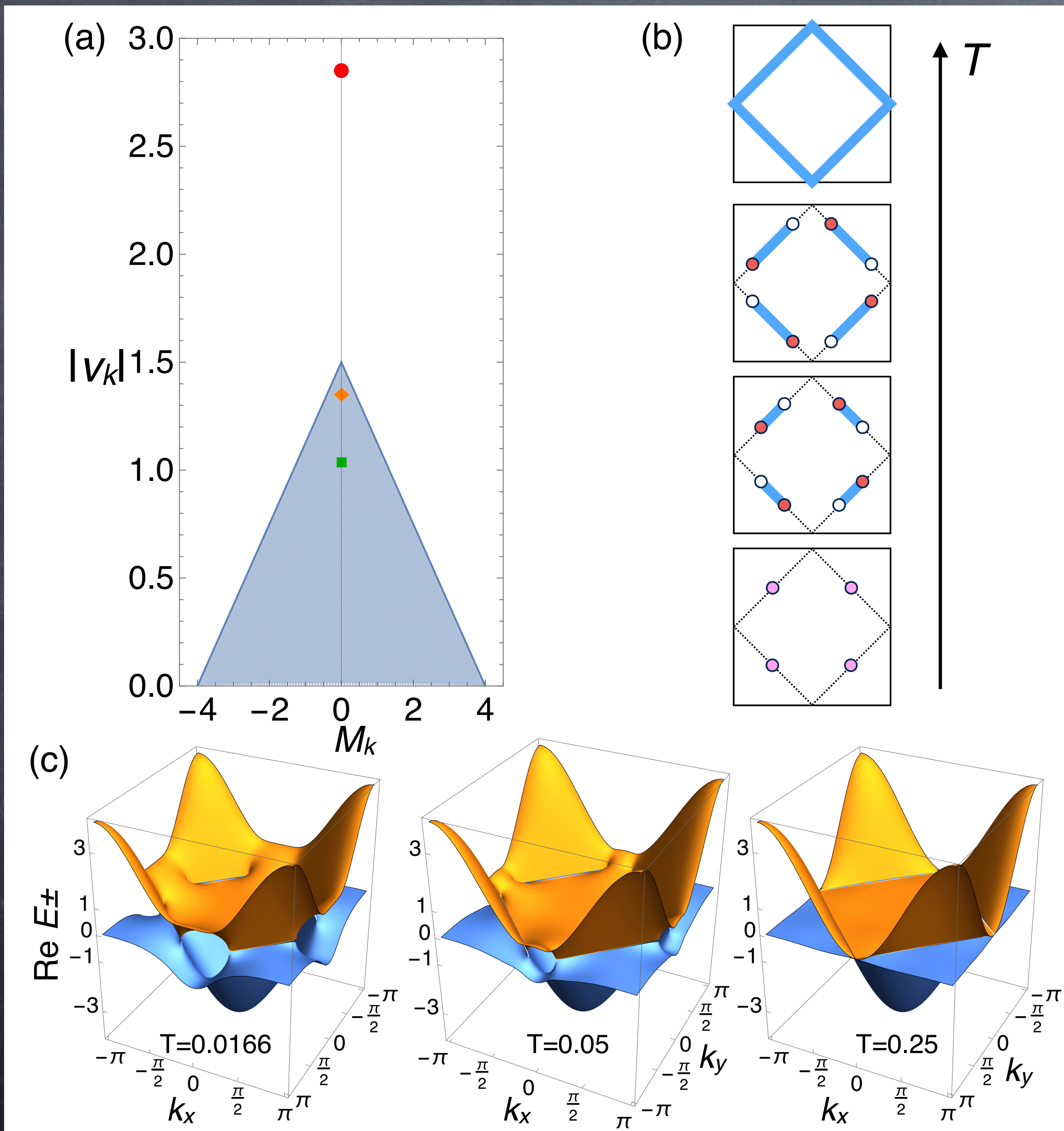
Periodic Anderson Model

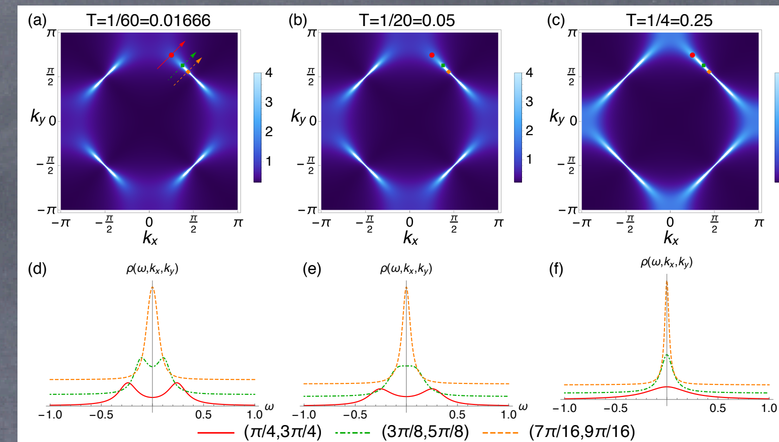
$$E_{\pm}(\mathbf{k},\omega) = \pm\frac{1}{2}\sqrt{(M_{\mathbf{k}} - i\Gamma)^2 + 4\,|\,v_{\mathbf{k}}\,|^2} + \frac{1}{2}(\epsilon_{f\mathbf{k}} - i\Gamma + \epsilon_{c\mathbf{k}})$$





DMFT results



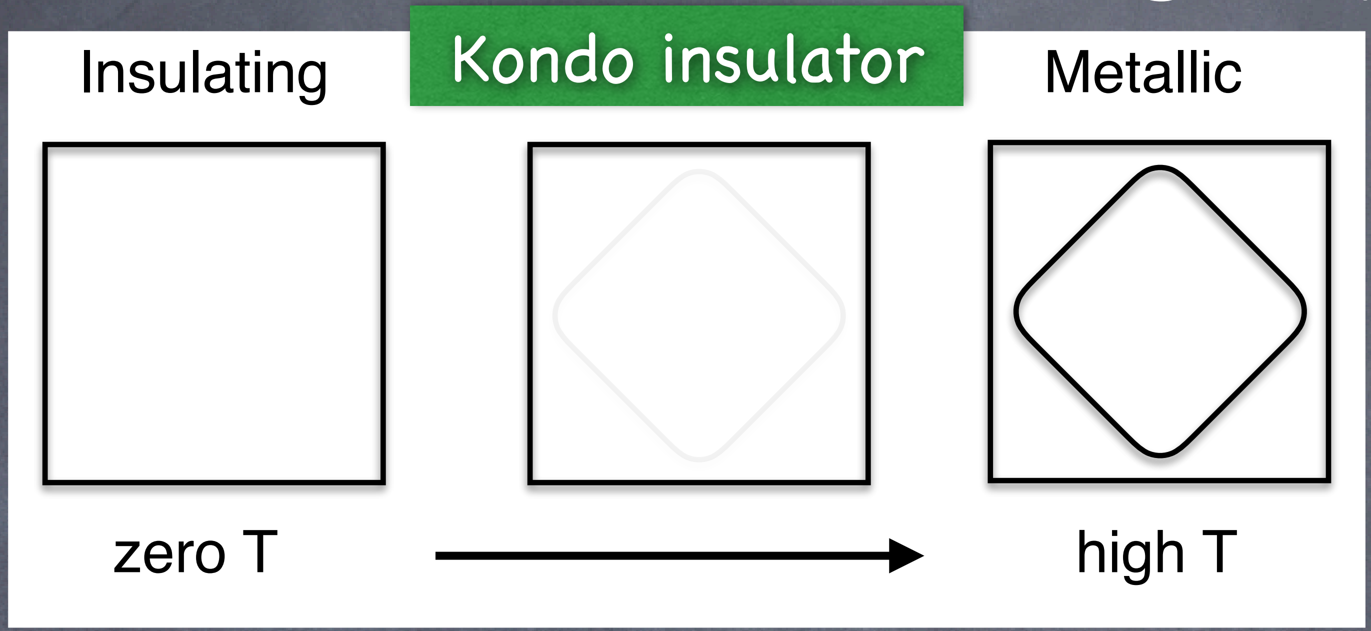


Exceptional points move with changing temperature

EPs marge and vanish at a boundary

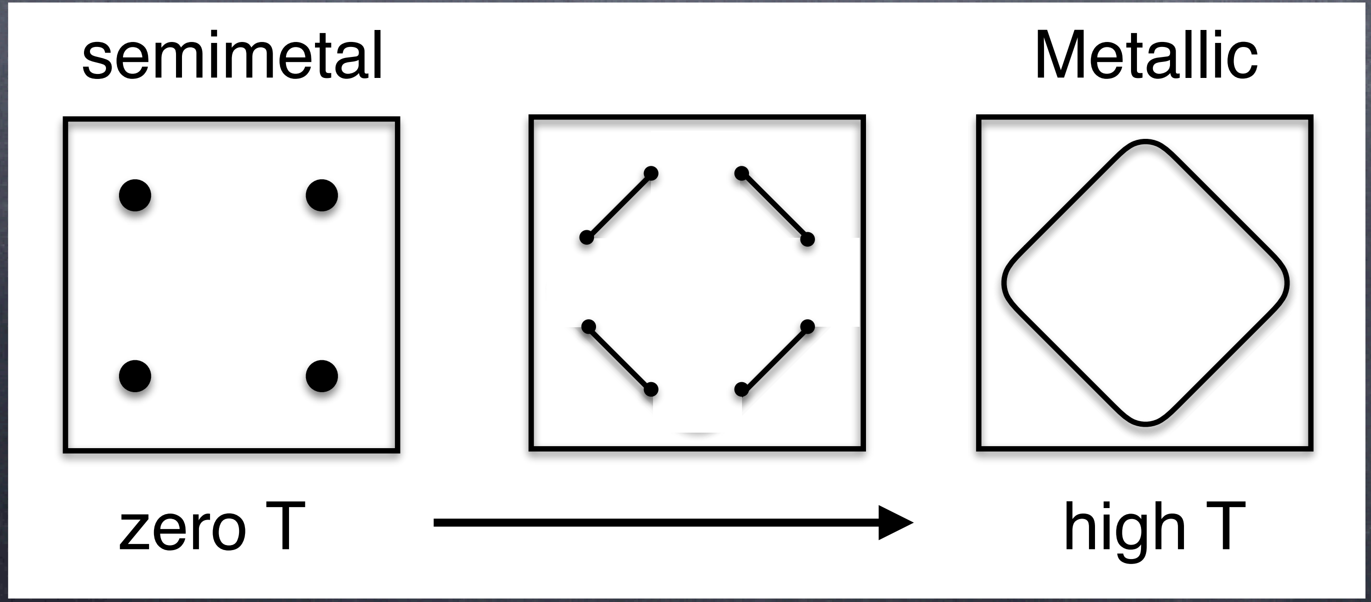
Bulk Fermi arcs appear in Kondo semimetal!

Explanation without using topology

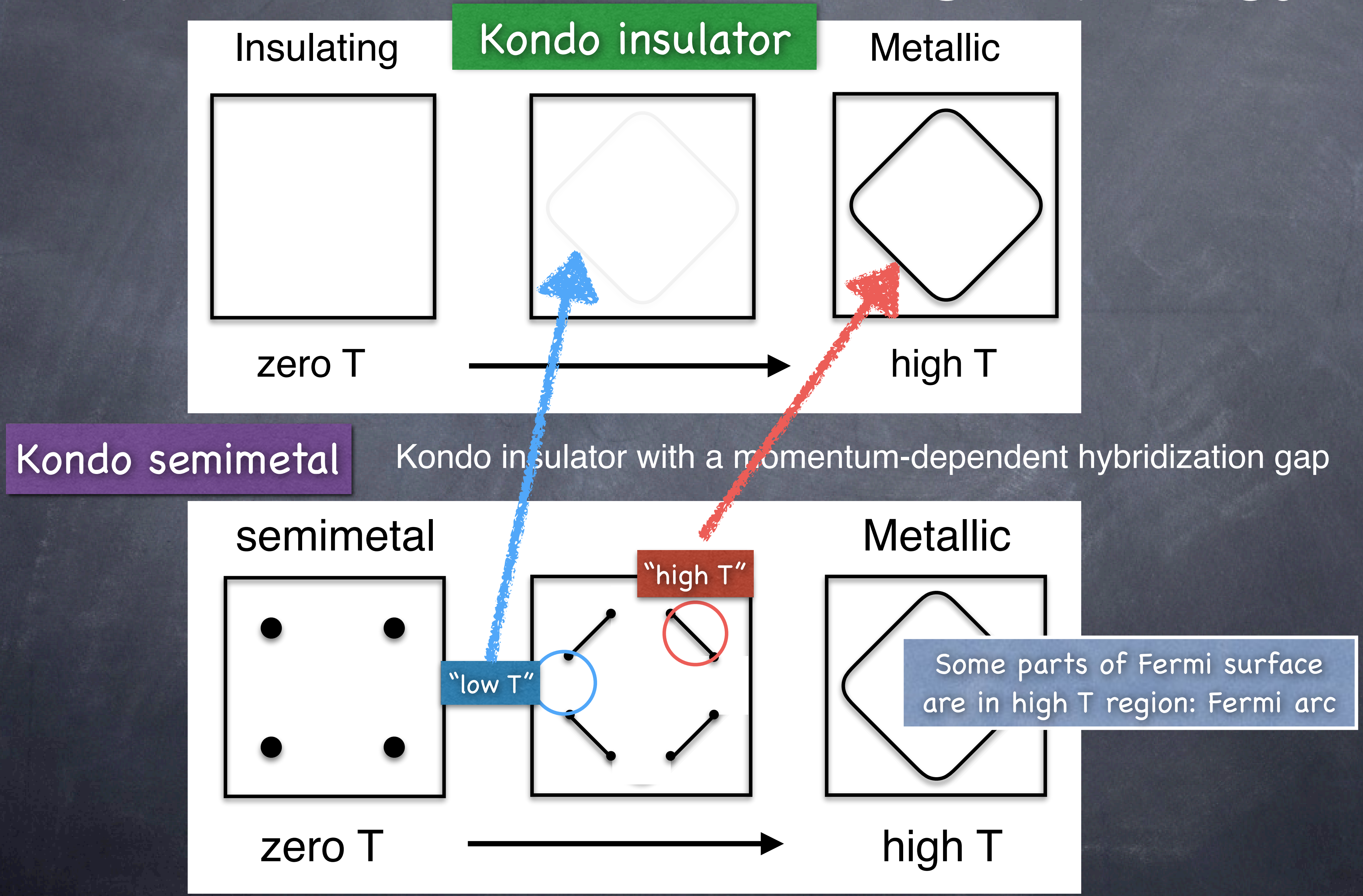


Kondo semimetal

Kondo insulator with a momentum-dependent hybridization gap



Explanation without using topology

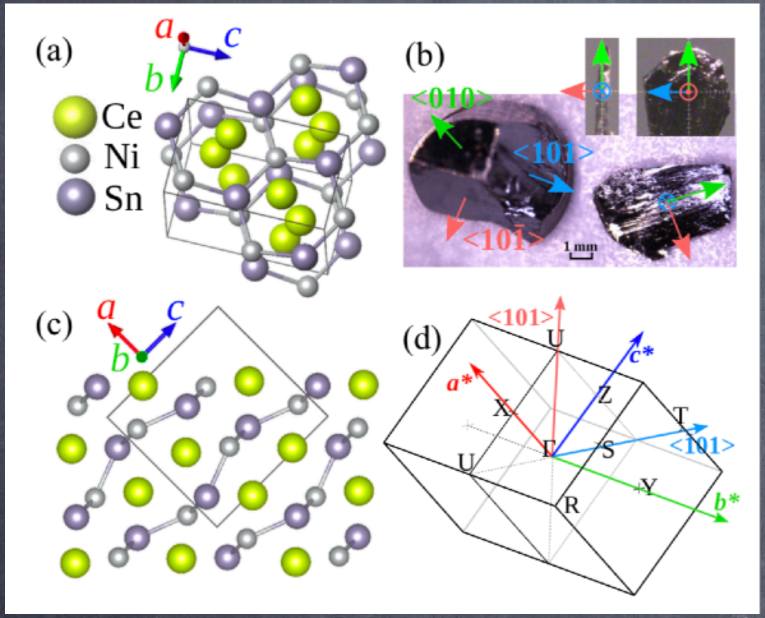


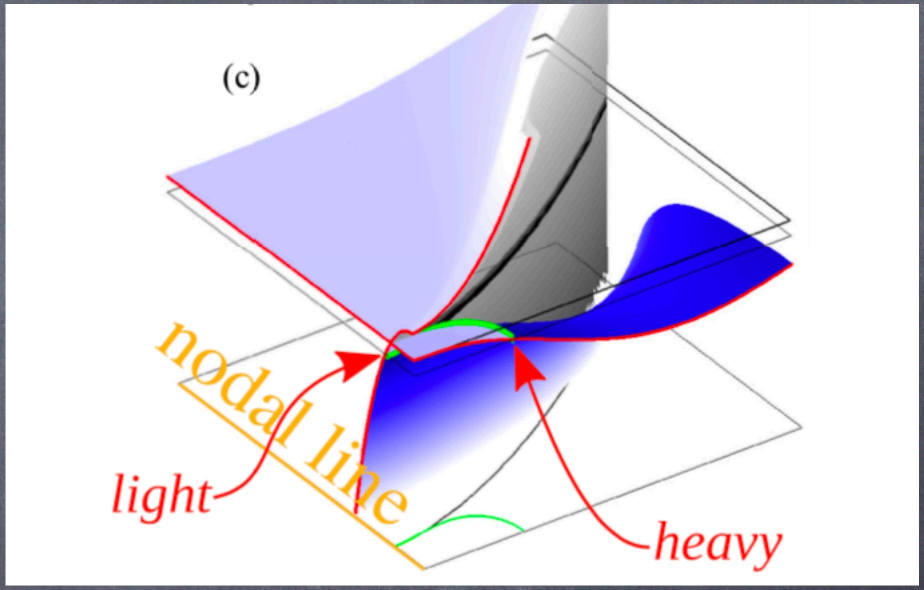
Kondo insulator with a momentum-dependent hybridization gap

Experiments: candidates?

CeNiSn: Kondo semimetal

C. Bareille, Phys. Rev. B 100, 045133 (2019)





ARPES experiment T = 12K

I discussed with this group in ISSP in Univ. of Tokyo

In lower temperatures, can we find Fermi arc?

Summary

Summary

Topological exceptional points can appear in heavy fermion systems

We used DMFT and found a bulk Fermi arc

Kondo semimetal can have a bulk Fermi arc

Quasiparticle Hamiltonian: $H(\mathbf{k},\omega) \equiv H_0(\mathbf{k}) + \Sigma(\mathbf{k},\omega)$

Topology in finite temperatures!

Yuki Nagai, Yang Qi, Hiroki Isobe, Vladyslav Kozii, and Liang Fu, to be appeared